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ADMISSIBILITY CRITERIA FOR
PROPAGATING PHASE BOUNDARIES IN
A van der WAALS FLUID

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ABSTRACT

^ This paper gives admissibility criteria for weak solutions to the
partial differentials equations governing isothermal motion of a van der
Waals fluid. The main issue is that an admissibility criterion based on
viscosity alone is too restrictive - it rules out all slowly propagating
phase boundaries. Instead a criterion based on viscosity and capil-
larity is proposed. The viscosity-capillarity condition is studied and
shown to imply that the state on one side of a phase boundary specifies
both the speed of the phase boundary and the state on the other side of
the phase boundary (a result which is differ.nt from classical gas
dynamics). ◄ ───

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Key Words: Phase transitions, viscosity criterion, viscosity-
              capillarity criterion, propagating phase boundary,
              van der Waals fluid

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SIGNIFICANCE AND EXPLANATION

Typically real fluids exhibit the property that under different configurations of pressure, density, temperature they can exist in different phases. For example water may exhibit vapor, liquid, and ice phases. Classical thermodynamics usually studies the co-existence of phases at equilibria so the term "thermodynamics" in this sense is a misnomer. In this paper the problem of true dynamic phase transitions is studied. In particular conditions are given for the existence of a propagating phase boundary separating liquid and vapor phases. The results are also applicable to phase transitions in solids undergoing "martensitic" or "shape-memory" phase transitions.

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CONTENTS

ADMISSIBILITY CRITERIA FOR PROPAGATING PHASE BOUNDARIES IN A van der WAALS FLUID

M. Slemrod

0. INTRODUCTION

The purpose of this paper is to present admissibility criteria for weak solutions to the equations governing isothermal motion of a van der Waals fluid. The idea of admissibility criteria is quite well known in the study of hyperbolic conservation laws (see for example Lax [1],[2]). However for the case of a van der Waals fluid the balance laws of linear momentum and conservation of mass lead to a mixed hyperbolic - elliptic initial value problem. Thus new issues appear which are not present in classical hyperbolic equations of inviscid compressible fluid dynamics.

The most obvious difficulty with a mixed hyperbolic - elliptic initial value problem is the classical Hadamard instability of solutions lying in the unstable elliptic regime. To circumvent this difficulty it is natural then to consider only initial value problems where the data is given in the stable hyperbolic domains. Thus we should expect to find "weak" or "generalized solutions" to the equations of motion where such solutions take on values only in the stable hyperbolic domains. These weak solutions will in general possess propagating singular surfaces separating states in one hyperbolic domain from states in another hyperbolic domain. These singular surfaces are called propagating phase boundaries. The question then becomes one of knowing in what sense such phase boundaries are admissible.

Two admissibility criteria are discussed here. The first
is a standard viscosity criterion. This will be discarded as too
                                            slowly
restrictive: it rules out all/propagating phase boundaries. The

second is a viscosity-capillarity condition . It allows for

propagating phase boundaries to exist but only in very special

cases. Namely for a propagating phase boundary to be admissible

according to the viscosity-capillarity condition the state on

one side of the phase boundary will determine both the propaga-

tion speed and the state on the other side of the boundary.

While this paper is devoted to fluid dynamics, the issues

involved are quite similar to those discussed in a recent paper

of James [3]. In that paper James has studied propagating phase

boundaries in one-dimensional non-linear elasticity where the

choice of constitutive relation leads to a mixed hyperbolic-

elliptic initial value problem similar to the one studied here.

Hence it may be that a criterion analagous to the viscosity-

capillarity condition may prove useful in elasticity as well as

fluid dynamics.

1. One dimensional Lagrangian description of compressible fluid
   flow

   We follow the presentation of Courant & Friedrichs [4] of
a Lagrangian description based on the law of conservation of mass.
The fluid flow is thought of taking place in a tube of unit cross
section along the x-axis. We attach the value X=0 to any definite
"zero" section moving with the fluid. For any other section we
let X be equal in magnitude of the mass of the fluid in the tube
of unit cross section area between that section and the zero
section. Analytically the quantity X satisfies the relation

$$X = \int_{X(o,t)}^{X(X,t)} \rho(x,t)\,dx.$$

Here $\rho(x,t)$ denotes the density at position x and time t and $x = X(X,t)$ denotes the position of the particle which encloses a
mass X of fluid in the tube bounded by $X(X,t)$ and $X(0,t)$. Dif-
ferentiation of (1.1) implies $1 = X_X(X,t)\rho(X X,t),t)$. Set
$\rho(X X,t),t) = \tilde{\rho}(X,t)$, $w(X,t) = \tilde{\rho}(X,t)^{-1}$ (the specific volume), $\dot{X}(X,t) = u(X,t) = X_t(X,t)$ (the velocity).

   We denote the stress by τ, the specific internal energy
by $\dot{\epsilon}$, the specific heat absorption by q, the heat flux by h, and
the specific body force by b. Then the equations of balance of
linear momentum, energy, and mass become

$$\rho\, \ddot{x} = \tau_x + \rho b \quad,$$

$$\rho\, \dot{\epsilon} = \rho q + \tau \dot{x}_x + h_x \quad,$$

$$\dot{\rho} + \rho \dot{x}_x = 0 \quad,$$

where $\cdot = \dfrac{d}{dt}$. We now apply the chain rule and rewrite this
system in terms of the independent variables X,t to obtain

$$X_{tt} = \tau_X + b \quad ,$$

$$\varepsilon_t = q + \tau X_{tX} + h_X \quad , \qquad\qquad (1.1)$$

$$(\tilde{\rho} X_X)_t = 0$$

where we have used the fact that $\dot{\rho}(x,t) = \tilde{\rho}_t(X,t)$. The third of these equations is automatically satisfied since $\tilde{\rho} X_X = 1$.

The above set of balance laws must be supplemented by constitutive relations. We assume the fluid is compressible and thermo-elastic so that the stress, internal energy, heat flux satisfy

$$\tau = \hat{\tau}(w,T) \quad ,$$

$$\varepsilon = \hat{\varepsilon}(w,T) \quad ,$$

$$h = \hat{h}(w,T,T_X) \quad ,$$

Furthermore we assume for simplicity that the fluid is imbedded in a "heat bath" so that the motion is isothermal (T=positive constant) and there are no body forces. Mathematically this means (i) that q in (1.1.b) is assumed to be adjusted so (1.1.b) will always be satisfied identically and (ii) b=0. In this case (1.1) equivalent to the first order system

$$u_t = \tau_X \quad ,$$

$$\qquad\qquad (1.2)$$

$$w_t = u_X \quad .$$

A C^1 curve $\Gamma : X = \gamma(t)$ across which u,w experience jumps is called a <u>singular surface</u>. If Γ is a singular surface let $(\gamma(\bar{t}),\bar{t})$ be a fixed point on the graph of Γ and $U = \dot{\gamma}(\bar{t})$. Denote by $u_+, w_+, u_- w_-$ the respective limits from the right and left as $(X,t) \to (\gamma(\bar{t}),\bar{t})$ for u,w. If we put $[u] = u_+ - u_-$, $[w] = w_+ - w_-$, etc.

then classically we know the Rankine-Huginot jump conditions must be satisfied, i.e.

$$U[u] + [\tau] = 0 \quad,$$
$$U[w] + [u] = 0 \quad.$$

(1.3)

Of course (1.3) implies U^2 satisfies the equation

$$U^2 = \frac{[\tau]}{[w]} \quad.$$

(1.4)

As we shall always be working on a fixed isotherm let us set $\hat{\tau}(w,T) = - p(w)$. In this case (1.2) becomes

$$u_t = - p(w)_x \,,$$
$$w_t = u_x \quad.$$

(1.5)

As is easily seen (1.5) is either hyperbolic or elliptic depending on the sign of $p'(w)$.

It is well known that conservation laws of the form (1.5) do not in general admit smooth solution. Typically discontinuities (shocks) will form in a finite time even for smooth initial data. Hence we must be satisfied solving (1.5) in the sense of distributions. Such solutions are termed weak solutions. Unfortunately as is also well known weak solutions are not generally uniquely determined by their initial values. To pick out the physically relevant ones some additional principle must be introduced. It is this issue which is pursued in the next sections.

2. Admissibility with respect to the viscosity criteron

Let us imbed the inviscid equations (1.6) in a viscous formulation, i.e. we take

$$\tau = - p(w) + \mu(w) u_X \quad . \tag{2.1}$$

Typically (see [1]) we like to know that if $u(X,t;\mu)$, $w(x,t;\mu)$ sequence of solutions to (1.2), (2.1) which tend to a limit $u(X,t;0)$, $w(X,t;0)$ boundedly, almost everywhere as $\mu(w) \to 0+$, then the limit functions $u(X,t;0)$, $w(X,t;0)$ satisfy (1.5) in the sense of distributions. In order to be sure that the term $(u(w)u_X)_X$ entering (1.2a) does indeed converge to zero as $\mu \to 0+$ in the distributional sense we require $\mu(w) = \mu_0$, a positive constant.

Now let $\Gamma : \quad X = \gamma(t)$ be a singular surface for (1.5). We now ask the question: Are solutions of (1.5) in the neighborhood of the singular surface Γ limits of solutions (1.2),(2.1) as $\mu_0 \to 0+$? While this problem has a history dating back to Rayleigh [5] it is the more recent discussions of Wendroff [6] and Dafermos [7] we shall follow.

Let $(\gamma(\bar{t}),\bar{t})$ be a fixed point on the graph Γ and let $u_+, w_+, u_-, w_-,$ U be as in Section 1. We look for a traveling wave solution of (1.2),(2.1) given by

$$u(X,t) = \hat{u}(\xi) \quad , \quad w(X,t) = \hat{w}(\xi) \quad , \quad \xi = \frac{X-Ut}{\mu_0} \quad .$$

It follows that $\hat{u}, \hat{w}$ must satisfy

$$- U\hat{u}' = (-p + \hat{u}')'$$

$$- U\hat{w}' = \hat{u}'$$

where $'$ denotes $\frac{d}{d\xi}$.

In order for $\hat{u}, \hat{w}$ to approximate the discontinuous profile of the solution to (1.6) we require

$$(\hat{u}(-\infty), \quad \hat{w}(-\infty), \quad \hat{u}(+\infty), \quad \hat{w}(+\infty)) = (u_-, w_-, u_+, w_+) \ . \qquad (2.3)$$

The above considerations motivate the following definition.

Definition 2.1 If there exists $\hat{u}, \hat{w}$ so that (2.2), (2.3) are satisfied for all points $(\gamma(\bar{t}), \bar{t})$ we will say the singular surface Γ satisfies the <u>viscosity admissibility criterion</u>.

Theorem 2.2 The viscosity admissibility criterion is satisfied if and only if

$$- U^2 + \left(- \frac{p(\bar{w}) + p(w_-)}{\bar{w} - w_-} \right) \geq 0 \ (\leq 0) \quad \text{if} \quad U > 0 \ (< 0) \qquad (2.4)$$

for every value $\bar{w}$ between w_- and w_+. In other words for $(w_+ - w_-) U > 0$ (or $(w_+ - w_-) U < 0$) the chord which joins $(w_-, p(w_-))$ to $(w_+, p(w_+))$ lies above (below) the graph of the function $p(w)$ for $\bar{w}$ between w_- and w_+.

Proof While proofs are presented in [6] and [7] we shall provide one for completeness.

Integrate (2.2) from $-\infty$ to ξ. It follows that

$$- U(\hat{u}(\xi) - u_-) = - p(\hat{w}(\xi)) + p(w_-) + \hat{u}'(\xi) \ ,$$
$$- U(\hat{w}(\xi) - w_-) = \hat{u}(\xi) - u_- \ , \qquad (2.5)$$

which it turn yields the first order equation

$$U^2(\hat{w}(\xi) - w_-) + p(\hat{w}(\xi)) - p(w_-) = - U \hat{w}'(\xi) \ . \qquad (2.6)$$

If $w_- < w_+$ then we must have $w'(\xi) > 0$ and hence, (2.4) follows. A similar argument is used if $w_+ < w_-$.

3. The van der Waals equation of state

On a fixed isotherm the van der Waals equation of state reads

$$\tilde{p}(w) = \frac{RT}{w-b} - \frac{a}{w^2} , \quad 0 < b < w < \infty , \qquad (3.1)$$

where a,b,R,T are all positive constants ([8],[9]). Pictorially $\tilde{p}(w)$ is represented in Fig. 1. if T is sufficiently small. As we shall not need anything so specific as (3.1) in our analysis let us suppose in what follows that $p(w)$ has basically the same type of graph as in Fig. 1, namely,

(i) $\quad p'(w) < 0 \qquad 0 < b < w < w_\alpha , \quad w_\beta < w ;$

(ii) $\quad p'(w_\alpha) = p'(w_\beta) = 0 ; \qquad\qquad (3.2)$

(iii) $\quad p'(w) > 0 \quad \text{if} \quad w_\alpha < w < w_\beta .$

The domains (b,w_α) and (w_β,∞) will be called the α-phase and β-phase respectively. The α-phase corresponds to the fluid being liquid, the β-phase corresponds to the fluid being vapor.

Definition 3.1 A singular surface Γ will be called a phase boundary (shock) if for every point on Γ w_+,w_- lie in different (the same) phase.

Theorem 3.2 For p satisfying (3.2) no phase boundary is admissible according to the viscosity criterion (Defn. 2.1) if $|U|$ is sufficiently small.

Proof The chord joining $(w_-,p(w_-))$ to $(w_+,p(w_+))$ must cut the graph of $p(w)$ and hence the viscosity criterion cannot be satisfied.

Since no slow phase boundaries are admissible according to the viscosity criterion it seems worthwhile to consider a less severe admissibility criterion. Indeed it may be that other

higher order effects other than viscosity should be considered.
One such effect that is particularly pronounced in the liquid-
vapor interface will be capillarity. A theory of interfacial
capillarity was proposed in [10] by Korteweg and a discussion
of his theory may be found in the monograph of Truesdell and
Noll [11]. Korteweg's theory has most recently been reconsidered
by Serrin [12] who has applied it to study condition for equili-
brium between liquid and vapor phases in a van der Waals fluid.
(A related theory based on statistical mechanics has been pre-
sented in [13]).

According to Korteweg's theory the stress τ in our one-
dimensional Lagrangian formulation will be given by

$$\tau = - p(w) + D(w)w_X^2 - C(w)w_{XX} + \mu(w)u_X \quad . \qquad (3.3)$$

As in the discussion of constitutive relation (2.1) we would
like to know that solutions of (1.2),(3.3) which tend to a limit
boundedly, almost everywhere, as $\mu(w) \to 0+$, $D(w) \to 0$, $C(w) \to 0$, will
converge to solutions of (1.5). So in order to be sure that
extra terms in (1.2),(3.3) due to the consideration of viscosity
and capillarity tend to zero in the sense of distributions as
$\mu(w) \to 0+$, $D(w) \to 0$, $C(w) \to 0$, we set

$$C(w) = \mu_0^2 A \quad ,$$
$$D(w) = 0 \quad , \qquad (3.4)$$
$$\mu(w) = \mu_0 \quad .$$

Thus in this special case (1.2),(3.3) becomes

$$u_t = (-p(w) - \mu_0^2 A w_{XX} + \mu_0 u_X)_X \quad , \qquad (3.5)$$
$$w_t = u_X \quad .$$

Now let Γ be a phase boundary and $\gamma(t)$, u_+, w_+, u_-, w_- U be
as in Section 1. Again we look for a traveling wave solution

$$u(X,t) = u(\xi) \quad , \quad w(X,t) = w(\xi) \quad , \quad \xi = \frac{X - Ut}{\mu_0} \quad .$$

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From (3.5) it then follows that $\hat{u}, \hat{w}$ must satisfy

$$- U\hat{u}' = (-p(\hat{w}) - A\hat{w}'' + \hat{u}')' \ ,$$

$$- U\hat{w}' = \hat{u}' \ . \tag{3.6}$$

So that $\hat{u}, \hat{w}$ will approximate the discontinuous profile of the solution to (1.5) we require

$$(\hat{u}(-\infty), \ \hat{w}(-\infty), \ \hat{u}(+\infty), \ \hat{w}(+\infty)) = (u_-, w_-, \ u_+, w_+) . \tag{3.7}$$

These considerations motivate the following definition.

<u>Definition 3.3</u> If there exsists $\hat{u}, \hat{w}$ so that (3.6),(3.7) are

satisfied for all points $(\gamma(\bar{t}), \bar{t})$ we will say the singular

surface Γ satisfies the <u>viscosity-capillarity</u> <u>admissibility</u>

<u>condition</u>.

For w_-, U (w_+, U) given in the α-phase (β-phase) let $w_+(U)$

$(w_-(U))$ denote the solution (if it exists) of

$$U^2 = - \frac{[p]}{[w]} \tag{3.8}$$

lying in the β-phase (α-phase). Also set

$$f_-(\zeta;U) = U^2(\zeta - w_-) + p(\zeta) - p(w_-) \ ,$$

$$f_+(\zeta;U) = U^2(\zeta - w_+) + p(\zeta) - p(w_+) \ .$$

Integration of (3.6) for $-\infty$ to ζ and the obvious substi-

tution shows a solution $\hat{w}$ of (3.6),(3.7) must satisfy the

second order equation

$$A\hat{w}'' + U\hat{w}' + f_-(\hat{w};U) = 0 \tag{3.9}$$

with boundary conditions

$$\hat{w}(-\infty) = w_-, \quad \hat{w}(+\infty) = w_+ \ . \tag{3.10}$$

<u>Lemma 3.4</u> Assume $A > 0$.

(i)   Let w_- be given and assume

$$(\mathrm{I}) \quad \int_{w_-}^{w_+(0)} f_-(\zeta;0)\,d\zeta < 0 \quad .$$

Then there exists a unique U*, $0 < U* < \overline{U}$, so that (3.9) possesses a solution with $w(-\infty) = w_-, w(+\infty) = w_+(U*)$. Here $\overline{U}$ is such that $\displaystyle\int_{w_-}^{w_+(\overline{U})} f_-(\zeta;\overline{U})\,d\zeta = 0.$

(ii)   Let w_+ be given and assume

$$(\mathrm{II}) \quad \int_{w_-(0)}^{w_+} f_+(\zeta;0)\,d\zeta > 0 \quad .$$

Then there exists a unique U*, $\overline{U} < U* < 0$, so that (3.9) possesses a solution with $w(-\infty) = w_-(U*)$, $w(+\infty) = w_+$. Here $\overline{U}$ is such that

$$\int_{w_-(\overline{U})}^{w_-} f_+(\zeta;\overline{U})\,d\zeta = 0 \quad .$$

Remark 3.5   The hypotheses of the lemma have a simple interpretation. For example in (i), (I) says that the signed area between the chord joining $(w_-,p(w_-))$ and $(w_+(0),p(w_+(0))$ and the graph of $p(w)$ between w_- and $w_+(0)$ is negative. $\overline{U}$ is that positive value of U so that the signed area between the chord joining $(w_-,p(w_-))$ and $(w_+(\overline{U}),p(w_+(\overline{U}))$ and the graph of $p(w)$ between w_- and $w_+(\overline{U})$ is zero (see Fig. 1). Analagous interpretations hold for (ii).

Proof of Lemma   (i)   Let $y(w(\xi)) = \hat{w}'(\xi)$.   Then (3.9) may be rewritten as

$$\frac{A}{2}\,\frac{d}{dw}\,y^2(w) + U\,y(w) + f_-(w;U) = 0.$$
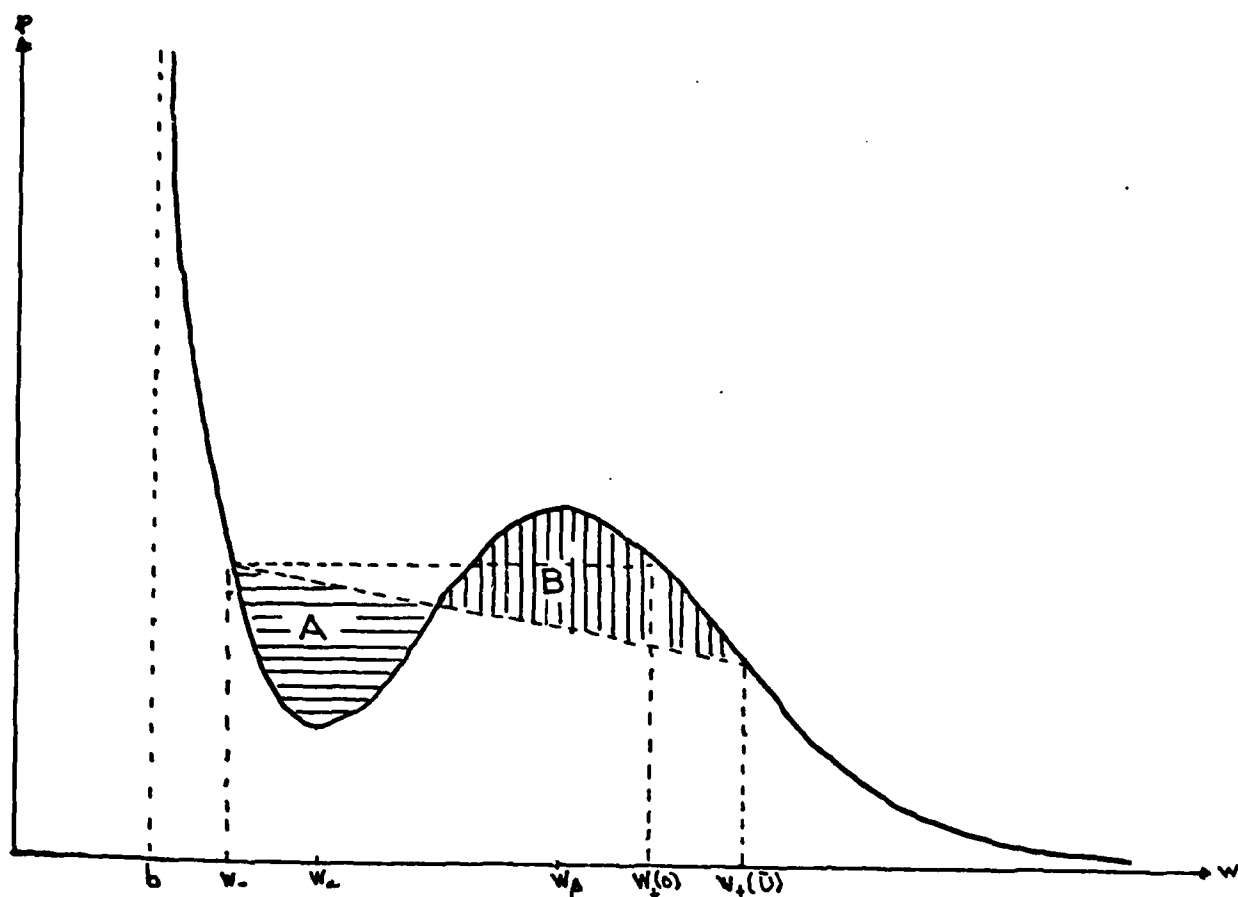
Integration from w_- to w yields

Figure 1   van der Waals   isotherm; w_- and $w_+(\overline{U})$ so that area
A = area B.

$$\frac{A}{2} y^2(w) = - U \int_{w_-}^{w} y(\zeta) \, d\zeta - \int_{w_-}^{w} f_-(\zeta; U) d\zeta \quad . \quad (3.11)$$

Let us now consider the case $U = 0$. Let $w^*(0)$ denote that value of w for which the chord connecting $(w_-, p(w_-))$ and $(w_+(0), p(w_+(0)))$ intersects the graph of $p(w)$, $w_\alpha < w^*(0) < w_\beta$. Since $f_-(\zeta, 0) > 0$ for $w^*(0) < \zeta < w_+(0)$ it follows that

$$\frac{A}{2} y^2(w) \geq - \int_{w_-}^{w_+(0)} f_-(\zeta; 0) d\zeta > 0$$

by (I). Hence if (I) holds and $U = 0$ the solution of (3.9) with $w(-\infty) = w_-$ always stays above the line $y = 0$.

Now let U increase from zero to $\overline{U}$. The solutions of (3.9) form a nested sequence in w-y plane; see Figure 2. By continuity with respect to the parameter U all that is needed to establish the existence of a unique U^* so that $w(+\infty) = w_+(U^*)$ is to show that the solution for $U = \overline{U}$ crosses the line $y = 0$. But from (3.11) we see

$$0 < \frac{A}{2} y^2(w_+(\overline{U})) = - \overline{U} \int_{w_-}^{w_+(\overline{U})} y(\zeta) d\zeta$$

So $y(\zeta)$ must go from positive to negative values for ζ between w_- and $w_+(\overline{U})$.

(ii) The proof is similar to (i).

Theorem 3.6 Assume $A > 0$,

(u_-, w_-) $((u_+, w_+))$ is to be a state to the left (right) of a point $(\gamma(\overline{t}), \overline{t})$ on a phase boundary Γ and the hypothesis I (II) of Lemma 3.4 holds. Then Γ is an admissible phase boundary according to the viscosity-capillarity condition if
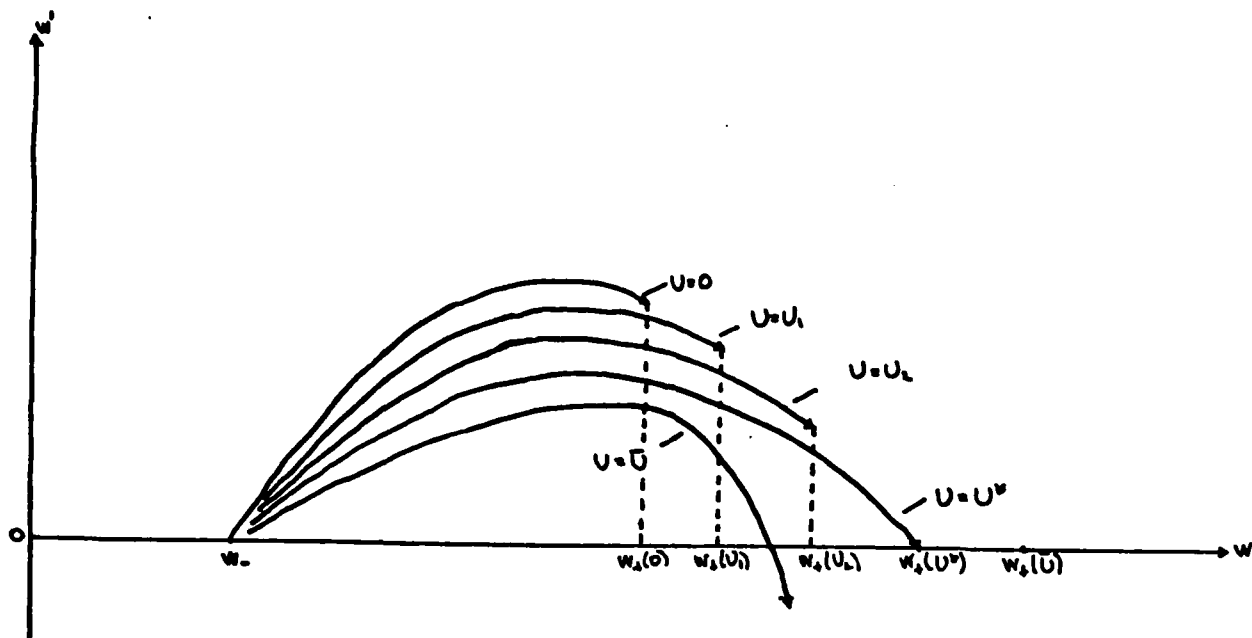
Figure 2 Phase plane plot of solutions of (3.9) for w_- fixed and U increasing zero, $0 < U_1 < U_2 < U^* < \bar{U}$.

and only if

$w_+ = w_+(U^*), \quad u_+ = u_- - U^*(w_+(U^*) - w_-),$

$\dot{\gamma}(t) = U^* > 0 \quad (w_- = w_-(U^*), \quad u_- = u_+ + U^*(w_+ - w_-(U^*))),$

$\dot{\gamma}(t) = U^* < 0$ where U^* and $w_+(U^*)$ (U^* and $w_-(U^*)$) are given by Lemma 3.4 (i) ((ii)).

Proof The result follows immediately from Lemma 3.4 and the Rankine-Huginot jump conditions (1.3).

Corollary 3.7 Let Γ be a singular surface (either shock or phase boundary) which is admissible according to the viscosity-capillarity condition for some $A > 0$. Let u_+, w_+, u_-, w, U be as in Section 2. Then the "entropy" inequality

$$U \left\{ \int_{w_-}^{w_+} p(\zeta) d\zeta - (w_+ - w_-) \frac{(p(w_+) + p(w_-))}{2} \right\} < 0 \qquad (3.12)$$

is satisfied. That is to say: U times the signed area between the graph of $p(\zeta)$ between w_- and w_+ and chord joining $(w_-, p(w_-))$ to $(w_+, p(w_+))$ is negative.

Proof If there is a solution $\hat{w}(\xi)$ to $(3.9'), (3.10)$ then multiplication of (3.9) by $\hat{w}'(\xi)$ yields

$$\frac{d}{d\zeta} \left\{ \frac{A}{2} \hat{w}'(\xi)^2 + \int_{w_-}^{\hat{w}(\xi)} f_-(\zeta; U) d\zeta \right\} = - U \hat{w}'(\xi)^2 \qquad (3.13)$$

Integration of (3.13) from $-\infty$ to ∞ implies

$$\int_{w_-}^{w_+} f_-(\zeta; U) d\zeta = - U \int_{-\infty}^{\infty} \hat{w}'(\xi)^2 d\xi,$$

or

$$U \int_{w_-}^{w_+} f_-(\zeta; U) d\zeta < 0. \qquad (3.14)$$

The integral indicated in (3.14) is precisely the bracketed expression in (3.12).

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While we have argued that the choice $\mu(w) = \mu_0$, $D(w) \equiv 0$, $C(w) = \mu_0^2 A$ is a natural assumption from the computational viewpoint one might still question whether the results of Theorem 3.6 carry over to a more general case. The answer is yes and is provided by the following result.

Assume $\mu(w) = \epsilon\mu_0(w)$, $C(w) = \epsilon^2 C_0(w)$, $D(w) = \epsilon^2 D_0(w)$ where $\epsilon > 0$ and $\mu_0(w) > \bar{\mu}_0 > 0$, $C_0(w) > \bar{C}_0 > 0$; $\bar{\mu}_0$, $\bar{C}_0$ constants. In this case (1.2),(3.3) becomes

$$u_t = (-p(w) + \epsilon^2 D_0(w)w_X^2 - \epsilon^2 C_0(w)w_X^2 + \epsilon\mu_0(w))_X \ ,$$

$$w_t = u_X \ . \tag{3.15}$$

Set $\xi = (\frac{X-Ut}{\epsilon})$ and $u = \hat{u}(\xi)$, $w = \hat{w}(\xi)$. It follows that $\hat{u}(\xi), \hat{w}(\xi)$ satisfy

$$- U\hat{u}' = (-p(\hat{w}) + D_0(\hat{w})\,\hat{w}'^2 - C_0(\hat{w})\,\hat{w}'' + \mu_0(\hat{w})\hat{u}')'$$

$$- U\hat{w}' = \hat{u}' \tag{3.16}$$

where we again impose boundary conditions (3.7). Integration of (3.16) from $-\infty$ to ξ implies

$$C_0(\hat{w})\hat{w}'' + U\mu_0(\hat{w})\hat{w}' - D_0(\hat{w})\hat{w}'^2 + p(\hat{w}) - p(w_-) - U^2(\hat{w}-w_-)=0 \tag{3.17}$$

we have boundary conditions (3.10). We now state the following generalization of Lemma 3.4.

Lemma 3.8

(i) Let w_- be given and assume

$$(\mathrm{I}') \qquad \int_{w_-}^{w_+(0)} \exp\left(2 \int_{\eta}^{w_+(0)} D_0(\zeta)C_0(\zeta)^{-1}d\zeta\right) C_0(\eta)^{-1}f_-(\eta;0)d\eta < 0$$

and that there exists $\bar{U} > 0$ so that

$$\int_{w_-}^{w_+(\bar{U})} \exp\left(2 \int_{\eta}^{w_+(0)} D_0(\zeta)C_0(\zeta)^{-1}d\zeta\right) C_0(\eta)^{-1}f_-(\eta;\bar{U})d\eta = 0 \ .$$

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Then there exists a unique U^*, $0 < U^* < \overline{U}$, so that (3.17) possesses a solution with $w(-\infty) = w_-$, $w(+\infty) = w_+(U^*)$.

(ii) Let w_+ be given and assume

(II*) $\int_{w_-(0)}^{w_+} \exp\left(2 \int_\eta^{w_-(0)} D_0(\zeta)C_0(\zeta)^{-1}d\zeta\right) C_0(\eta)^{-1} f_+(\eta;0)\,d\eta > 0$

and that there exists $\overline{U} < 0$ so that

$\int_{w_-(\overline{U})}^{w_+} \exp\left(2 \int_\eta^{w_-(0)} D_0(\zeta)C_0(\zeta)^{-1}d\zeta\right) C_0(\eta)^{-1} f_+(\eta;\overline{U})\,d\eta = 0$.

Then there exists a unique U^*, $\overline{U} < U^* < 0$, so that (3.17) possesses a solution with $w(-\infty) = w_-(U^*)$, $w(+\infty) = w_+$.

The proof is similar to the proof of Lemma 3.4 and is omitted.

4. Relation to the Lax shock criterion

In this section we compare the viscosity-capillarity admissibility condition to the well known Lax shock criterion ([1],[2]) in the case $p' < 0$, i.e. (1.6) is strictly hyperbolic.

Definition 4.1 For system (1.6) with $p' < 0$ we shall say a shock $\Gamma : X = \gamma(t)$ joining states $(u_+, w_+), (u_-, w_-)$ at $(\bar{t}, \gamma(\bar{t}))$ satisfies the <u>Lax shock condition</u> if either

$$(-p'(w_+))^{\frac{1}{2}} < U < (-p'(w_-))^{\frac{1}{2}}$$

or

$$-(-p'(w_+))^{\frac{1}{2}} < U < -(-p'(w_-))^{\frac{1}{2}}$$

where $U = \dot{\gamma}(\bar{t})$.

Theorem 4.1 If $p' < 0$ and $p'' \neq 0$ a shock Γ which is admissible according to the viscosity-capillarity condition for any $A > 0$ is admissible according to the Lax shock condition.

Proof In this case (3.9) possesses two equilibrium points $(w_-, 0)$ and $(w_+, 0)$. If we know there is a connecting orbit for $U > 0$ then either $(w_-, 0)$ and $(w_+, 0)$ are both saddles or $(w_-, 0)$ is a saddle and $(w_+, 0)$ is stable node. The condition $p'' \neq 0$ and linearization about $(w_-, 0)$ shows the two saddle case is impossible. Finally it follows easily that saddle-node case implies the Lax shock condition. The case $U < 0$ is proved in the same way.

Theorem 4.2 If $p' < 0$ and $p'' > 0$ a shock wave Γ which is admissible according to the Lax shock criterion is admissible according to the viscosity-capillarity condition for any $A > 0$.

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__Proof__ Consider the case $(-p'(w_+))^{\frac{1}{2}} < U < (-p'(w_-))^{\frac{1}{2}}$; the other

case is analagous. Let $A > 0$ be fixed and let

$$V(\hat{w},\hat{w}') = \frac{A\hat{w}'^2}{2} + \int_{w_-}^{\hat{w}} f_-(\zeta;U)\,d\zeta .$$

Since $p'' > 0$ we have $V \to \infty$ as $|(\hat{w},\hat{w}')| \to \infty$ and

$$\frac{dV}{d\zeta}(\hat{w},\hat{w}') = - U w'(\zeta)^2 \leq 0$$

along solutions of (3.9). Then all orbits are bounded in the

(w,w') plane and by LaSalle's Invariance Principle [14] they

must approach an equilibrium. These facts combined with

Lemma 4.1 of [15] yield the theorem.

5. An elementary Riemann problem for a van der Waals fluid.

Consider (1.6) where $p(w)$ has graph similar to that of Fig. 1, i.e. p satisfies (3.2). The Riemann initial value problem consists of specifying initial conditions

$$u = u_0 \atop w = w_0 \quad , \quad X<0; \qquad u = u_1 \atop w = w_1 \quad , \quad X>0, \quad u_0, u_1, w_0, w_1 \text{ constants.} \quad (5.1)$$

In this section we consider the special choice of data u_0, w_0, u_1, w_1 so that w_0 is in the α-phase, w_1 is in the β-phase and u_0, w_0, u_1, w_1 satisfying Rankine-Huginot jump conditions for some U. This of course implies $p(w_0) > p(w_1)$ if $w_0 < w_1$, $p(w_0) < p(w_1)$ if $w_0 > w_1$. It is a trivial observation that

$$u = u_0 \atop w = w_0 \quad , \quad X<Ut; \qquad u = u_1 \atop w = w_1 \quad , \quad X>Ut \qquad\qquad (5.2)$$

is a weak solution of (1.6),(5.1). The sign of U is as of yet undetermined. The line $X=Ut$ is a phase boundary. From our previous results we can then conclude the following

<u>Theorem 5.1</u> The phase boundary $X = Ut$ in the solution (5.2) of

(1.5),(5.1),(3.2) is inadmissible according to the viscosity

criterion (Definition 2.1). If $w_- = w_0$ satisfies (I) of Lemma

3.4 there is a unique $U^* > 0$, $w_1 = w_+(U^*)$, $u_1 = u_0 - U^*(w_+(U^*)-w_-)$,

so that $X = U^*t$ is an admissible phase boundary according to

the viscosity-capillarity condition. If $w_+ = w_1$ satisfies (II)

of Lemma 3.4 there is a unique $U^* < 0$, $w_0 = w_-(U^*)$, $u_0 = u_1 +$

$U^*(w - w_-(U^*))$, so that $X = U^*t$ is an admissible phase boundary

according to the viscosity-capillarity condition.

Thus while (5.1) provides infinitely many possible solutions to a Riemann problem for (u_0, w_0) fixed and (u_1, w_1) allowed to vary, the viscosity-capillarity conditions says that solutions of the form (5.2) will be allowed only for one choice of (u_1, w_1) if w_0 satisfies (I) of Lemma 3.4. Of course a similar statement holds if w_1 satisfies (II) of Lemma 3.4.

6. A possible experimental method for computing the coeffi-
cient A in Korteweg's theory.

In the preceding section we have seen that under certain
conditions for a given A in the capillarity formulae (3.3),(3.4)
a propagating phase boundary will be admissible with a certain
speed U*. This result then presents an inverse problem. Con-
sider an experiment in which a propagating phase boundary is
observed for a van der Waals type fluid. Can one find an A
so that the theory of Section 3 matches the experiment? If one
can find such an A (possibly using numerical integration of
(3.9)) then an estimate of the coefficient A is obtained.

In constrast to the above dynamic experiment an observation
of a steady state phase boundary ($\dot{\gamma}(t) \equiv 0$) will not provide an
identification of A. For if $\dot{\gamma}(t) \equiv 0$
have $p(w_-) = p(w_+)$ and from (3.9) we have

$$\int_{w_-}^{w_+} (p(\zeta) - p(w_-))d\zeta = 0 \tag{6.1}$$

for all choices of A > 0. Of course (6.1) is just a statement
of Maxwell's equal area rule [8],[9],[12]. The point here is
that calculating the non-zero speed of propagation of a phase
boundary can provide an estimate of A; such a determination
will not follow from studying a steady state phase boundary.

Needless to say the above discussion has the implicit
premise that the coefficient D in Korteweg's theory is zero. This
may or may not be the case. If D $\equiv$ 0 (6.1) shows the Maxwell
equal area rule holds. However the converse is not true. Serrin

has shown in [12] that the equal area rule may hold even for non-zero D. Hence experimental knowledge of the equal area rule's applicability for a given fluid would not in itself imply $D \equiv 0$. The converse is true, however, i.e. if the equal area rule does not hold for phase equilibrium then $D \neq 0$. This follows immediately from the remarks preceding (6.1). Of course in such cases as $D \neq 0$, and for more general choices of $\mu(w)$, $C(w)$, Lemma 3.8 may prove of value in parameter identification.

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References

1. P. Lax, Shock waves and entropy in Contributions to Non-linear Functional Analysis, E. Zarantonello, editor, Academic Press: New York, London (1971), 603-634.

2. P. Lax, Hyperbolic systems of conservation laws and the mathematical theory of shock waves, CBMS Regional Conference Series in Applied Mathematics, SIAM Publications: Philadelphia (1973).

3. R.D. James, The propagation of phase boundaries in elastic bars, Archive for Rational Mechanics and Analysis, 73, (1980), 125-158.

4. R. Courant and K.O. Friedrichs, Supersonic Flow and Shock Waves, John Wiley, Intersciences: New York (1948).

5. Lord Rayleigh, Aerial plane waves of finite amplitude, Proc. Royal Society of London, Series A, 84, (1910), 247-284.

6. B. Wendroff, The Riemann problem for materials with nonconvex equations of state, J. Mathematical Analysis and Applications, 38, (1972), 454-466.

7. C.M. Dafermos, The entropy rate admissibility criterion in thermoelasticity, Rendiconti della Classe di Scienze fisiche, matematiche e naturali, Accademi Nazionale dei Lincei, Serie VII, LVII, (1974), 113-119.

8. A.B. Pippard, Elements of Classical Thermodynamics, Cambridge University Press: Cambridge (1964).

9. A. Sommerfeld, Thermodynamics and statistical mechanics, Academic Press: New York and London, (1964).

10. D.J. Korteweg, Sur la forme que prennent les equations du mouvement des fluides si l'on tient compte des forces capillaires par des variations de densite, Archives Neerlandaises des Sciences exactes and Naturelles, Series II, 6, (1901), 1-24.

11. C.A. Truesdell and W. Noll, The non-linear field theories of mechanics, Vol. III/3 of the Encyclopedia of Physics, S. Flugge, editor, Springer-Verlag: Berlin(1965).

12. J. Serrin, Phase transitions and interfacial layers for van der Waals fluids, to appear in Proc. of SAFA IV Conference, Recent Methods in Nonlinear Analysis and Applications, Naples, March 21-28, 1980, A. Canfora, S. Rionero, C. Sbordone, C. Trombetti, editors.

References

13. V. Bongiorno, L.E. Scriven, and H.T. Davis, Molecular
    theory of fluid interfaces, Journal of Colloid and
    Inferface Science, 57, (1976), 462-475.

14. J.K. Hale, Ordinary differential equations, Krieger
    Publishing Co: Huntington, NY (1980).

15. C.C. Conley and J.A. Smoller, Viscosity matrices for two-
    dimensional nonlinear hyperbolic systems, Comm. Pure and
    Applied Mathematics, XXIII, (1970), 867-884.

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This paper gives admissibility criteria for weak solutions to the partial differentials equations governing isothermal motion of a van der Waals fluid. The main issue is that an admissibility criterion based on viscosity alone is too restrictive - it rules out all slowly propagating phase boundaries. Instead a criterion based on viscosity and capillarity is proposed. The viscosity-capillarity condition is studied and shown to imply that the state on one side of a phase boundary specifies both the speed of the phase boundary and the state on the other side of the phase boundary (a result which is different from classical gas dynamics).

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